Fact Sheet

MODELING THE TRANSPORT OF HEAVY METALS IN SOILS MRTM (MULTI-REACTION AND TRANSPORT MODEL)

PROBLEM

To protect groundwater, you must be able to predict the movement of heavy metals in soils. Prediction of potential groundwater contamination has considerable health implications and is necessary for cleanup of former disposal sites. Mathematical models to describe movement of heavy metals in soils must include information on both retention and transport of metals in soil.

SOLUTION

We examined various models predicting transpor and retention of metals in soils. From these we developed four general-purpose multi-reaction, multi-site, kinetic-based computer simulation models. These models were rigorously tested, with extensive evaluation of variables in a range of soils.

- MRM is a multi-reaction model that includes concurrent and concurrent-consecutive retention processes of the nonlinear kinetic type. It accounts for equilibrium (Freundlich) sorption and irreversible reactions. The processes considered are based on linear (first-order) and nonlinear (second-order) kinetic reactions. MRM can describe heavy metals under batch conditions where water flow is not considered.
- MRTM is a multi-reaction and transport model. It is an extension of MRM, with the retention processes
 incorporated into the convection-dispersion equation for solute transport in soils under steady water
 flow.
- SOTS is a second-order kinetic approach for describing solute retention during transport in soils. It
 accounts for sites on the soil matrix that can retain the reactive solutes in solution. It assumes these
 processes are predominantly controlled by surface reactions of adsorption and exchange. The secondorder reactions associated with the two sites may be considered as kinetically controlled, heterogeneous chemical retention reactions.
- SOMIM extends the second-order model of the diffusion-controlled mobile-immobile or two-region
 concept. It assumes the retention process is controlled by two types of reactions: a chemically controlled heterogeneous reaction and a physically controlled reaction. The first is governed by the secondorder approach, the second by diffusion or mass transfer of the mobile-immobile concept. Irreversible
 reaction of the first-order kinetic type was also incorporated in the transport model.

PRODUCTS AVAILABLE

- Computer program and sample input/output runs for each model for all DOS-based personal computers (5.25" or 3.5" disks).
- Selim, H.M., M.C. Amacher, and I.K. Iskandar (1990) Modeling the transport of heavy metals in soils. CRREL Monograph 90-2, U.S. Army CRREL, Hanover, New Hampshire.

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